A return to observability near exceptional points in a schematic $\mathcal{PT}$−symmetric model

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Abstract

Many indefinite-metric (often called pseudo-Hermitian or $\mathcal{PT}$−symmetric) quantum models H prove "physical" (i.e., Hermitian with respect to an innovated, *ad hoc* scalar product) inside a characteristic domain of parameters $\mathcal{D}$. This means that the energies get complex (= unobservable) beyond the boundary $\partial\mathcal{D}$ (= Kato's "exceptional points", EPs). In a solvable example we detect an enlargement of $\mathcal{D}$ caused by the emergence of a new degree of freedom. We conjecture that such a beneficial mechanism of a return to the real spectrum near EPs may be generic and largely model-independent.

1 Introduction and summary

Over virtually any model in quantum phenomenology one initially feels urged to consider *all* the relevant degrees of freedom in the corresponding Langangian $\mathcal{L}$ or Hamiltonian $\mathcal{H}$. This tendency is limited by the imperatives of the tractability of calculations and of a feasibility of making measurable predictions. Thus, for example, for an electron moving in a very strong external Coulomb field, an exhaustive theoretical analysis requires the full-fledged formalism of relativistic quantum field theory but some of the measurable properties of the bound states are still very satisfactorily predicted by the mere quantum-mechanical, exactly solvable Dirac-equation model [1].

One of the most characteristic features of many "reduced" models of the latter type is that their reliability (i.e., in an abstract formulation, the negligibility of relevance of their "frozen" degrees of freedom) may vary with some of their dynamical parameters. Thus, in the same illustration one reveals that when the external field becomes strong enough, some of the Dirac-field-excitation components of the system enter the scene and become directly coupled to the motion of the electron itself [1]. In such a dynamical regime the Dirac-equation predictions fail and, formally and typically, the energies of the electron itself become complex.

On a simplified model-building level the similar "paradoxes" in the behavior of the energies may be explained using the parity-pseudo-Hermitian Hamiltonians H. They are often called $\mathcal{PT}-$symmetric, with the defining property $H \neq H^\dagger = \mathcal{T} H \mathcal{T} = \mathcal{P} H \mathcal{P}$ and with a formal operator-conjugation $\mathcal{T}$ mimicking the time reversal and with $\mathcal{P}$ representing the parity (cf. also Appendix A for more details).

The latter Hamiltonians still can be re-interpreted as self-adjoint (i.e., observable) but one must restrict their set of dynamical parameters (i.e., of couplings etc) to a certain subdomain $\mathcal{D}^{(physical)}$ on which their spectrum remains real. In the context of Quantum Mechanics, more details may be found in the review paper [2], while an immediate and inspiring extension of such a recipe to Field Theory has only been proposed much more recently, in ref. [3].

In our recent letter [4] we introduced, for illustrative purposes, a two-state model with the generic one-parametric $\mathcal{PT}-$symmetric Hamiltonian

$$H^{(2)} = \begin{pmatrix} -1 & a \\ -a & 1 \end{pmatrix}, \qquad \mathcal{P}^{(2)} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1}$$

We also explained there the existence of a nontrivial formal relationship between our simple model (1) and its more standard (and phenomenologically ambitious) differential-operator predecessors or analogues $H^{(\mathcal{PT})}$ (say, of refs. [5]). In essence, this relationship is based on the replacement of $H^{(\mathcal{PT})}$ by their equivalent infinite-dimensional matrix representants $H^{(\infty)}$ (in a suitable basis) and, subsequently, by their variational, $N-$dimensional truncated-matrix approximants $H^{(N)}$ with $N < \infty$. In such a context it still makes sense to coin the name "parities" for the corresponding "indefinite-metric" matrices $\mathcal{P}^{(N)}$ which enter the finite-dimensional pseudo-Hermiticity property $H^\dagger \mathcal{P}^{(N)} = \mathcal{P}^{(N)} H$ of the matrix toy Hamiltonians $H = H^{(N)}$.

The key purpose of our present short paper is to show that the simple matrix models of the form (1) can say a lot about the interpretation of the general $\mathcal{PT}-$symmetric Hamiltonians in the critical regime where their energies are about to complexify. In this sense we intend to complement now our remark [4] on the schematic model $H^{(2)}$ by a few new and interesting observations based on a tentative immersion of the two-dimensional system in a generic three-dimensional one,

$$H^{(3)} = \left(\begin{array}{cc|c} -1 & a & 0 \\ -a & 1 & b \\ \hline 0 & -b & 3+c \end{array} \right) \qquad \mathcal{P}^{(3)} = \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array} \right). \qquad (2)$$

Here, the standard Jacobi rotation has been employed in setting zeros in the corners of $H^{(3)}$ so that the three-parametric example (2) preserves the full generality of its one-parametric predecessor (1).

In a continuation of the study [4] we shall be able to show that and how a fairly satisfactory insight in several qualitative though, up to now, not too well understood properties of the general $\mathcal{PT}-$symmetric models can be deduced from the mere comparison of the virtually elementary models (1) and (2). First of all, such a comparison will enable us to study some of the aspects of the above-mentioned conflict between the use of the models with "too few" and "too many" degrees of freedom by choosing the models $H^{(2)}$ and $H^{(3)}$ as their respective representatives. In section 2 we emphasize that the vanishing of one of the two coupling constants in the "universal-like" model $H^{(3)}$ leads directly to the sample "reduced" model of the form $H^{(2)}$. A few relevant results on $H^{(2)}$ of ref. [4] are summarized there for the sake of completeness as well.

Our mathematical encouragement lies in the exact non-numerical tractability of the "universal" model $H^{(3)}$. In section 3 the feasibility of quantitative calculations

will enable us to extend the results of ref. [4] to the richer model $H^{(3)}$ where we set $c = 0$ for the sake of simplicity. In particular, we shall show that the formula for the boundary $\partial \mathcal{D}(H^{(3)})$ of the domain where all the energies remain real can be written in closed form.

A core of our message will be formulated in section 4 where we show how the growth of $\mathcal{D}(H^{(N)})$ from $N = 2$ to $N = 3$ shifts the Kato's exceptional points [6]. In subsection 4.1 we emphasize that in the closest vicinity of such an exceptional point at $N = 2$, even the weakest coupling to an "observer channel" induces a steady growth of the modified quasi-Hermiticity domain $\mathcal{D}(H^{(2)})$. In subsection 4.2, this observation is extended to the manifestly non-perturbative regime with the strongest couplings near the doubly exceptional points where all the three energy levels coincide.

One could summarize our present message as opening the possibility of a systematic amendment of various $\mathcal{PT}-$symmetric models near exceptional points via a re-activation of certain "frozen" degrees of freedom. In this sense, more work is still needed to confirm that our qualitative observations might stay valid far beyond the range of the present study.

Let us add that in Appendix A we complemented our discussion by a concise review of literature showing the physical background and, perhaps, broader relevance and possible impact of our schematic models. In a more technical remark of Appendix B we finally show that the role of $c \neq 0$ in our model $H^{(3)}$ can be rightfully ignored as not too essential.

2 Simulated changes of degrees of freedom

2.1 Decoupling an observer state: $b \to 0$ and $H^{(3)} \to H^{(2)}$

Once we start from the illustrative example (1), letter [4] tells us that

- the eigenenergies remain real and non-degenerate whenever $a^2 < 1$,

$$E_\pm = \pm\sqrt{1 - a^2}$$

  so that we may set $a = \cos\alpha$ with $\alpha \in (0, \pi)$ in $\mathcal{D}(H^{(2)})$;

- the necessary *ad hoc* scalar products of Appendix A are obtainable via a metric operator in (8). The choice of this operator is ambiguous, with its elements

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numbered by an overall multiplicative constant and by another real parameter $\gamma \in [0, \pi/2)$,

$$\Theta \sim \begin{pmatrix} 1 + \xi & -\cos \alpha \\ -\cos \alpha & 1 - \xi \end{pmatrix}, \qquad \xi = \sin \alpha \sin \gamma \, ; \tag{3}$$

- at *both* the exceptional points $\alpha^{(EP)} = 0, \pi$ of the boundary $\partial \mathcal{D}$, *all* the matrices $\Theta = \Theta(\gamma)$ cease to be invertible so that Θ^{-1} [needed in definition (9) below] ceases to exist.

One may note that at the EP singularities the geometric and algebraic multiplicities of eigenvalues become different. Some energies complexify immediately beyond these points. Near the points of the boundary $\partial \mathcal{D}$, all the predictions of quantum mechanics may be more sensitive to perturbations and must be examined particularly carefully.

2.2 A re-activated degree of freedom: $b \neq 0$ and $H^{(2)} \rightarrow H^{(3)}$

In the language of physics, one should contemplate introducing some new degree(s) of freedom near every exceptional point. The majority of the current Hamiltonians H [say, of the differential-operator form (10) discussed in Appendix A] does not offer a feasible option of this type. In contrast, the finite-dimensional matrix models can incorporate a new degree of freedom very easily, via an elementary increase of their dimension.

In an illustration let us first recollect that in the two-dimensional model of preceding paragraph we have $a^{(EP)} = \pm 1$. In the vicinity of these exceptional points we may set $a = \pm(1 - \varepsilon)$ with a real and sufficiently small ε which remains positive inside $\mathcal{D}(H^{(2)})$, vanishes in the EP regime and gets negative outside the domain.

An increase of the dimension N in $H^{(N)}$ from 2 to 3 should be accompanied by a coupling of the submatrix $H^{(2)}$ to a new, "observer" element of the basis. The resulting $\mathcal{PT}-$symmetric three-state matrix model (2) contains a new real coupling b and another real parameter $c \neq -2, -4$. Note that the presence of the two vanishing elements in $H^{(3)}$ does not weaken its generality since the corresponding two-by-two submatrix remains Hermitian and is assumed pre-diagonalized.

3 Exceptional points in the model $H^{(3)}$

A pairwise attraction of the energy levels mediated by the variations of the couplings a and b in $H^{(3)}$ should control the changes of the spectrum in full analogy with the generic two-state model. The role of the third parameter c is less essential and the discussion of its influence is postponed to Appendix B. Now we set $c = 0$ and insert our toy Hamiltonian (2) in the three-state Schrödinger equation. Its determinantal secular equation for energies

$$-E^3 + 3\,E^2 + \left(-a^2 + 1 - b^2\right) E - 3 + 3\,a^2 - b^2 = 0 \tag{4}$$

is solvable in closed form, via the well known Cardano formulae. Cardano formulae offer the roots of eq. (4) in the compact and non-numerical form which is, unfortunately, not too suitable for the specification of the domain $\mathcal{D}$. In a preparatory step, let us analyze a few simpler special cases of eq. (4), therefore.

3.1 Boundary $\partial\mathcal{D}$ at $a = c = 0$ or $b = c = 0$

A quick inspection of eq. (4) reveals that the cheapest information about $\partial\mathcal{D}$ becomes available when $ab = 0$. We choose $b = 0$ and decouple $H^{(3)} = H^{(2)} \oplus H^{(1)}$. The analysis degenerates to the two-dimensional problem and restricts the admissible values of a to the following open interval,

$$a \in \mathcal{D}|_{b=0} = (-1, 1).$$

This means that at $b = 0$ the "observer" level $E_2 = 3$ stays decoupled and it does not vary with a at all, while the two other levels (i.e., $E_0 = -1$ and $E_1 = 1$ at $a = 0$) become attracted in proportion to the strength $a \neq 0$ of the non-Hermiticity.

A completely analogous situation is encountered at $a = 0$. In this case it is comfortable to shift $E \to E - 2$ and get another section of quasi-Hermiticity domain in closed form,

$$b \in \mathcal{D}|_{a=0} = (-1, 1).$$

The genuine three-state phenomena may only occur when *both* a and b remain non-zero, making all the three energy levels *mutually* attracted.

3.2 The regime of simultaneous attraction, $a \neq 0 \neq b$

The set of the exceptional points forms the boundary $\partial \mathcal{D}$ which connects the above-mentioned four exceptional points in the $a - b$ plane. Its shape (see Figure 1) may be deduced from secular eq. (4) by a "brute-force" numerical technique. There also exists its non-numerical description replacing the non-degenerate triplet of energies E by the doubly degenerate energy $z = 1 + \beta$ *plus* a separate, "observer" third energy value $y = -1 + 2\alpha$.

In the case of $b > a > 0$ the value of z should result from a merger of $E_1 = 1$ with $E_2 = 3$ so that we may expect that $\beta \in (0, 1)$. Similarly, one may discuss the other orderings of a and b. In parallel, the necessary universality of the attraction of the levels (as observed above in the two-dimensional model) implies that we must always have $\alpha > 0$. Thus, once we replace eq. (4) by its adapted polynomial EP version of the same (third) degree in E,

$$-(E - z)^2 (E - y) = -E^3 + (2z + y)\, E^2 - \left(z^2 + 2yz\right) E + yz^2 = 0 \qquad (5)$$

the comparison of the quadratic terms in these two alternatives gives us the constraint $\alpha + \beta = 1$. Similarly, the reparametrization of the linear and constant contributions leads to the set of the two equations

$$a^2 + b^2 = 4 - 3\beta^2, \qquad 3a^2 - b^2 = 4 - 3\beta^2 - 2\beta^3$$

which may be re-read as the desired one-parametric definition of the star-like shape of the curve forming the boundary $\partial \mathcal{D}(H^{(3)})$, with $\beta \in (-1, 1)$,

$$a = a_\pm = \pm \sqrt{\frac{1}{2} (4 - 3\beta^2 - \beta^3)}, \quad b = b_\pm = \pm \sqrt{\frac{1}{2} (4 - 3\beta^2 + \beta^3)}. \qquad (6)$$

We may notice that all the four above-mentioned special EP cases are reproduced by this formula at $\beta = \pm 1$. Our analytic description of the boundary $\partial \mathcal{D}(H^{(3)})$ at $c = 0$ is complete.

4 Beneficial effects of the growth of $b \neq 0$

Having the parametric definition (6) of boundary $\partial \mathcal{D}(H^{(3)})$ at our disposal we know precisely where the energy spectrum remains real. This observation has several mathematically easy but physically appealing and relevant consequences.

4.1 A return of energies from complex to real

We originally started from the two-level model $H^{(2)}$ containing a single parameter a. This means that in the language of the "complete" three-state model $H^{(3)}$ we worked in the regime $b = 0$ where the "spectator" degree of freedom stayed decoupled. Critical EP values were $a = a^{(EP)} = \pm 1$ so that the energies lost their observability (i.e., the system collapsed) in arbitrarily small vicinities of these EPs.

The situation changes when the real and, say, not too large coupling $b \neq 0$ is switched on.

Lemma

Whenever our two-level model $H^{(2)}$ becomes coupled to a "spectator" state with $c = 0$ and $b \neq 0$ in $H^{(3)}$, energies remain real for $a \in (-1 - \eta, 1 + \eta)$ at certain $\eta = \eta(b) > 0$.

Proof

From the definition (6) we may infer that, say, near the EP where $(a, b) = (1, 0)$ we may set $\beta = -1 + \varepsilon^2 + \mathcal{O}(\varepsilon^3)$ and deduce that

$$b^{(EP)} = \sqrt{\frac{1}{2} [4 - 3(1 - 2\varepsilon^2) - (1 - 3\varepsilon^2) + \mathcal{O}(\varepsilon^3)]} = \frac{3\varepsilon}{\sqrt{2}} + \mathcal{O}(\varepsilon^2).$$

In parallel we have

$$a^{(EP)} = \sqrt{\frac{1}{2} [4 - 3(1 - 2\varepsilon^2) + (1 - 3\varepsilon^2) + \mathcal{O}(\varepsilon^3)]} = 1 + \frac{3\varepsilon^2}{4} + \mathcal{O}(\varepsilon^3)$$

so that we come to the conclusion that the EP value of a grows with $|b|$,

$$a^{(EP)} = 1 + \frac{\left[b^{(EP)}\right]^2}{6} + \mathcal{O}\left\{\left[b^{(EP)}\right]^3\right\}.$$

This means that we are allowed to choose a positive $\eta(b) = \mathcal{O}(b^2)$.

QED.

We see that whenever we introduce a new "degree of freedom" by setting $b \neq 0$, our system becomes stable in a non-empty vicinity of any of the two original exceptional points $a = \pm 1$. In the light of a "generic" character of our example $H^{(3)}$, one may expect similar behaviour of parametric dependence of the reality of the spectrum in *all* the other (or at least "many") $\mathcal{PT}$−symmetric models, irrespectively of their particular matrix or differential-operator realization.

4.2 Doubly exceptional character of the strongest acceptable couplings

Due to the mutual attraction of the energy levels in our "generic" three-by-three example one may expect that there exist certain "doubly exceptional" points (DEPs) of the boundary $\partial \mathcal{D}(H^{(3)})$ where *all* the three energies coincide at a triple root $E = z$ of the secular equation,

$$(E - z)^3 = 0 . \tag{7}$$

The comparison of the coefficients in eqs. (4) and (7) at E^2 gives $z = 1$. The subsequent two comparisons provide the two other coupled polynomial equations,

$$-3 = 1 - a^2 - b^2, \qquad 1 = -3 + 3\,a^2 - b^2 .$$

We get quickly $b^2 = 4 - a^2$ from the first equation while the assignment $a^2 = 2$ follows from the second one, in agreement with eq. (6) at $\beta = 0$.

We may conclude that in the light of Figure 1 and formulae (6), the boundary of the domain $\mathcal{D}(H^{(3)})$ of the allowed real matrix elements a and b remains smooth not only in the perturbative vicinity of the four points of subsection 3.1,

$$(a, b) \in \{ (1, 0), (0, 1), (-1, 0), (0, -1) \},$$

but also at all the pairwise mergers of the real energies. The spikes are encountered at the four "maximal-coupling" vertices of a circumscribed square,

$$(a, b) \in \{ (\sqrt{2}, \sqrt{2}), (-\sqrt{2}, \sqrt{2}), (-\sqrt{2}, -\sqrt{2}), (\sqrt{2}, -\sqrt{2}) \}$$

where one locates the DEP triple-energy mergers. The fourfold symmetry of the whole boundary $\partial \mathcal{D}^{(3)}$ of the quasi-Hermiticity domain is just an accidental consequence of our simplifying choice of the vanishing spectral shift $c = 0$.

Acknowledgement

Figure captions

Figure 1. Domain of quasi-Hermiticity at $c = 0$

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Appendix A: A concise review of the origin of the present schematic model

The concept of quasi-Hermiticity has been introduced in nuclear physics [2] where variational calculations of complicated nuclei proved facilitated by the replacement of the common inner product $\langle \psi | \phi \rangle$ in Hilbert space by its generalization

$$\langle \psi | \Theta | \phi \rangle \,, \qquad \Theta = \Theta^\dagger > 0 \,. \tag{8}$$

Indeed, quantum mechanics can be formulated using *any* invertible and positive definite metric operator Θ in (8). One can feel free to choose any nonstandard $\Theta \neq I$ and to select observables (i.e., Hamiltonians H etc) represented by operators which are Hermitian with respect to the new product (8). Whenever $\Theta \neq I$ we may call such observables *quasi-Hermitian*. In the language of algebra this means

$$H = H^\ddagger \;\equiv\; \Theta^{-1} H^\dagger \Theta \,. \tag{9}$$

This condition may be compatible with the manifest non-Hermiticity of H, provided only that the spectrum remains real. Incidentally, such a reality condition has been found satisfied by the quartic anharmonic oscillator "with wrong sign" [7] (in this case the coordinate ceases to be observable [8]) as well as by the "wrong-coupling" cubic oscillator [9] (in this model the non-observability concerns its purely imaginary potential [10]). Still, a real boom of interest in the manifestly non-Hermitian quantum Hamiltonians with real spectra has only been inspired by the well written letter by Bender and Boettcher in 1998 [11]. Very persuasive numerical and WKB arguments have been given there supporting the reality of spectrum for a broad class of Hamiltonians, with a remarkable impact on field theory [12].

The latter class involves the manifestly non-Hermitian one-dimensional models

$$H = -\frac{d^2}{dx^2} + U(x) + \mathrm{i}\, W(x) \neq H^\dagger \tag{10}$$

defined on $\mathbb{L}_2(\mathbb{R})$ and containing the two real components of the potential exhibiting the property called $\mathcal{PT}-$symmetry [7],

$$\mathcal{P}\, U(x)\, \mathcal{P}\; (\equiv\; U(-x)\;) = +U(x) \,, \qquad \mathcal{P}\, W(x)\, \mathcal{P} = -W(x) \,. \tag{11}$$

The rigorous proofs [13] of the reality of the spectra (or, in the present language, of the quasi-Hermiticity) of many non-Hermitian toy Hamiltonians $H \neq H^\dagger$ proved

complicated but the inconvenience has been circumvented by the turn of attention to exactly solvable $\mathcal{PT}$−symmetric potentials [14]. Their use simplified the proofs and mathematics but still, our understanding of the "correct" assignment of the physical interpretation to a given model remained incomplete [15]. Another simplifying reduction of the problem was needed and finite-dimensional matrix Hamiltonians entered the scene [16]. In particular, our recent discussion of the ambiguity of Θ [4] proved best illustrated by the replacement of both the $\mathcal{PT}$−symmetric Hamiltonian (10) and the operator of parity $\mathcal{P}$ by the mere two-dimensional, highly schematic matrices with real elements.

Appendix B: An irrelevance of the shift c

Even though we confirmed the fourfold symmetry of $\partial\mathcal{D}(H^{(3)})$ in paragraph 3.2, this symmetry must be interpreted as a mere artifact attributed to our choice of the most comfortable specific $c = 0$. Numerical experiments indicate that the curve $\partial\mathcal{D}(H^{(3)})$ gets deformed and distorted in proportion to the degree of violation of the equidistance of the diagonal matrix elements in $H^{(3)}$. Moreover, as long as all the $c \neq 0$ models (2) are characterized by a not too much more complicated secular equation

$$-E^3 + (3 + c)\,E^2 + \left(1 - a^2 - b^2\right)E - 3 + 3\,a^2 - c + ca^2 - b^2 = 0 \qquad (12)$$

it would still be feasible to quantify the effect non-numerically. The method employed in paragraph 4.2 remains applicable and it leads to an elementary shift of the DEP energy, $3z = 3 + c$. The parallel analytic analysis of the $c \neq 0$ problem is left to the reader. It remains straightforward though a bit boring. For example, in the most interesting triple-confluence regime the mere slightly more complicated pair of equations

$$-3 = 1 - a^2 - b^2, \qquad 1 = -3 + 3\,a^2 - c + ca^2 - b^2$$

gives the mere rescaled formulae which relate the DEP matrix elements in $H^{(3)}$,

$$a^2 = 2 - \frac{c}{4 + c} = 4 - b^2.$$

Obviously, the fourfold symmetry of Figure 1 will be broken in a way which is continuous in the limit of $c \to 0$.

Figure 1. Domain of quasi-Hermiticity at c=0